Electronic Supplementary Material (ESI) for Molecular BioSystems.
This journal is © The Royal Society of Chemistry 2014

## Supplementary file 2: The web server for GPCR prediction

As pointed out in [1] and emphasized in [2], user-friendly and publicly accessible web servers, which can significantly aid the research community, represent the future direction for developing practically more useful predictors, and we have established a web server for the new prediction method presented in this paper (http://genomics.fzu.edu.cn/GPCR/index.html). The server was designed using Java, Perl and HTML. The cores of Trans-GPCR, SSEA-GPCR and PPA-GPCR programs were developed using Java and can be run independently. The server does not require any additional information other than the target sequence itself. Users can submit multiple proteins to the server each time. For each protein, it is first iteratively threaded through local NCBI [3] NR database for three iterations to generate sequence profiles. The profiles are then fed into the Trans-GPCR to predict TM regions. Meanwhile, the target protein is judged whether it is GPCRs through Trans-GPCR by using TM region (i.e. *TransGPCR_Score* measure), SSEA-GPCR by using protein secondary structure topologies (i.e. *SSEA_gpcr* measure), and PPA-GPCR by using evolutionary relationship (i.e. *PPA_gpcr* measure). We use multi-thread technique to run the jobs. The computational time for finishing a job depends on the length of target sequence. It is estimated that a job will be finished within 10 minutes if the protein is less than 500 amino acids. The prediction results will be mailed to users when they are finished. Meanwhile, we also provide traceable accession numbers to users when they submit jobs. To maximize the performance of the web server, a regularly-updated library, which covers all sequence/structure spaces of known GPCRs is needed. To facilitate the users, the stand-alone programs can be downloaded from our web server and they can be run independently for high-throughput data.

## References

1. K. C. Chou and H. B. Shen, *Natural Science*, 2009, **1**, 63-92. doi: 10.4236/ns.2009.12011.
2. Lin, S. and Lapointe, J. *Journal of Biomedical Science and Engineering*, 2013,**6**, 435-442. doi: 10.4236/jbise.2013.64054.
3. K. D. Pruitt, T. Tatusova, W. Klimke and D. R. Maglott, *Nucleic acids research*, 2009, **37**, D32-36.